

12-ethyltricosane

Inchi:	InChI=1S/C25H52/c1-4-7-9-11-13-15-17-19-21-23-25(6-3)24-22-20-18-16-14-12-10-8-5-
InchiKey:	IDYSNLVYORVPBH-UHFFFAOYSA-N
Formula:	C25H52
SMILES:	CCCCCCCCCCCC(CC)CCCCCCCCCCC
Mol. weight [g/mol]:	352.68
CAS:	79370-85-7

Physical Properties

Property code	Value	Unit	Source
gf	157.18	kJ/mol	Joback Method
hf	-564.61	kJ/mol	Joback Method
hfus	56.98	kJ/mol	Joback Method
hvap	70.86	kJ/mol	Joback Method
log10ws	-10.05		Crippen Method
logp	9.854		Crippen Method
mcvol	363.110	ml/mol	McGowan Method
pc	767.34	kPa	Joback Method
rinpol	2405.00		NIST Webbook
rinpol	2414.00		NIST Webbook
rinpol	2405.00		NIST Webbook
tb	770.96	K	Joback Method
tc	944.71	K	Joback Method
tf	356.51	K	Joback Method
vc	1.429	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1151.89	J/molxK	770.96	Joback Method
cpg	1175.34	J/molxK	799.92	Joback Method
cpg	1197.69	J/molxK	828.88	Joback Method
cpg	1218.99	J/molxK	857.83	Joback Method
cpg	1239.27	J/molxK	886.79	Joback Method
cpg	1258.59	J/molxK	915.75	Joback Method

cpg	1276.97	J/molxK	944.71	Joback Method
dvisc	0.0027240	Paxs	356.51	Joback Method
dvisc	0.0007960	Paxs	425.58	Joback Method
dvisc	0.0003280	Paxs	494.66	Joback Method
dvisc	0.0001679	Paxs	563.73	Joback Method
dvisc	0.0000995	Paxs	632.81	Joback Method
dvisc	0.0000654	Paxs	701.88	Joback Method
dvisc	0.0000463	Paxs	770.96	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.97636e+01
Coeff. B	-1.01735e+04
Temperature range (K), min.	522.36
Temperature range (K), max.	703.94

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R248194&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions

h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀w_s:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
m_{cvol}:	McGowan's characteristic volume
p_c:	Critical Pressure
p_{vap}:	Vapor pressure
r_{inpol}:	Non-polar retention indices
t_b:	Normal Boiling Point Temperature
t_c:	Critical Temperature
t_f:	Normal melting (fusion) point
v_c:	Critical Volume

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